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Investigation of water displacement following large CO₂ sequestration operations

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Abstract

The scale of CO₂ injection into the subsurface required to address CO₂ atmospheric concentrations is unprecedented. Multiple injection sites injecting into multiple formations will create a large excess pressure zone extending far beyond the limited volume where CO₂ is present. In a closed system, additional mass is accommodated by the compressibility of system components, an increase in fluid pressure, and possibly an uplift of the land surface. In an open system, as assumed in this analysis, another coping mechanism involves fluid flux out of the boundaries of the system, in which case the fresh-water-bearing outcrop areas, corresponding to the up-dip sections of the down-dip formations into which CO₂ is injected, could be impacted. A preliminary study using a MODFLOW groundwater model extending far down-dip shows that injecting a large amount of fluid does have an impact some distance away from the injection area but most likely only in localized areas. A major assumption of this preliminary work was that multiphase processes do not matter some distance away from the injection zones. In a second step, presented in this paper, to demonstrate that a simplified model can yield results as useful as those of a more sophisticated multiphase-flow compositional model, we model the same system using CMG-GEM software. Because the chosen software lacks the ability to deal easily with unconfined water flow, we compare fluxes through time, as given by MODFLOW and CMG-GEM models at the confined/unconfined interface.

Keywords: pressure pulse, up-dip sections, evapotranspiration, stream leakage, MODFLOW.

1. Introduction

Injection of large amount of CO₂ in the subsurface without concomitant fluid production (as generally done in the oil and gas industry) has the potential to impact up-dip sections of the formations used for injection where they crop out, away from the injection area, and where they undergo recharge (Fig. 1). This paper investigates the possible impact of the pressure pulse traveling in the up-dip direction along the formation and affecting, by a domino effect, the fresh water zone which could see brackish water invasion. The large pressure pulse may also push saline water up leakage conduits (wells and faults), processes not considered in this paper. This research had two specific objectives: (1) quantify the impact of large-scale anthropogenic CO₂ injection on the fresh water section using site-specific information, and (2) determine the feasibility of using a simple single-phase flow code instead of a more complex multiphase flow code when modeling water displacement in the far-field.

Nicot [1] adapted a MODFLOW model developed to assess fresh water sources in aquifers of the upper Texas Gulf Coast (Fig. 2). The widely used code MODFLOW, regularly updated by the U.S. Geological Survey, is fundamentally a single phase code with no provision for variable-density flow. However with some simple modifications (Table 1), it may be able to provide relatively accurate pressure and flux values far away from the injection zone where the details of the origin of the pressure pulse are less important. In order to vindicate this fundamental assumption made in Nicot [1], we proceed in this paper to present some results obtained with CMG-GEM, a commercial compositional multi-phase flow numerical code initially designed for the oil and

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gas industry but also used in many instances in the field of geological carbon sequestration. Conclusions from the initial study (Nicot [1]) included the numerical observation that such massive injection should not impact much the fresh water zone on average but that in some instance the effect could be locally focused, in particular by the presence of flow barriers (such as the Mexia-Talco Fault zone just down-dip of the outcrop modeled in the Nicot [1] case study). For example, locally, the water table can rise several meters above their pre-development steady state level generating increased evapotranspiration and stream leakage and possible flooding of low-lying areas. However, the water table rise averages <1m (Nicot [1]).

This study, as well as Nicot [1]'s study, makes use of the Carrizo-Wilcox system (Fig. 2) which is a group of formations representative of the several sedimentary wedges of the Texas Gulf Coast that could provide large CO₂ storage capacity. The model represents the oldest of the stratigraphic wedges (Carrizo-Wilcox). The model was initially developed for determining regional water resources (Dutton et al. [2]), has been calibrated for that purpose, and includes a large down-dip section well beyond the volume containing fresh water. The (hypothetical) injection is done at a depth of 1.5 to 2 km (8,000 to 10,000 ft) in the Simsboro Formation through 50 wells injecting at a yearly rate of 1 million tons of CO₂, or equivalent CO₂, located at a variable distance from the outcrop but in the order of 100 km. It should be noted that we are not trying, in any case, to assess capacity of the Carrizo-Wilcox system. Because MODFLOW is a single-phase code, in this case, we injected a volume of water equivalent to the cumulative volume of CO₂ injected assuming a density of 700 kg/m³. The model abstracts the Carrizo-Wilcox as essentially five layers, each with a limited region of up-dip outcrop and an extended confined down-dip section of increasing thickness. Two major aquifers are modeled: the Carrizo and the deeper Simsboro aquifers. The top layer is a marine shale with little permeability. The two formations underlying the two aquifers are thick semi-confining unit with a large proportion of mudstones and local sandstones. All parameters (porosity, conductivity, top of formation, thickness of formation, and storativity) are distributed on a grid of 1-mi² (2.6-km²) cells. The modeled domain covers approximately 80,000 km². The model extends down-dip to the top of the so-called geopressured zone (Dutton et al. [3]) located at a depth of ~2,500 to 3,000 m within ~100 km of the outcrop area.

2. MODFLOW / CMG-GEM Input

To better compare results, MODFLOW and CMG-GEM models use the same basic grid: 5 layers of variable thickness and 273×177 1.609×1.609 km (1×1 mile) cells, not all of them active as can be seen on Fig. 2. Because CMG-GEM does not easily handle either unconfined conditions or shallow subsurface processes such as recharge, evapotranspiration (ET), and surface water – ground water interactions, the CMG-GEM grid stops at the last updip confined cell of the uppermost layer. In addition the injection layer was refined into 4 sublayers in CMG-GEM and injection is restricted to the bottom sublayer whereas the whole thickness of the Simsboro Formation is used in the MODFLOW model.

Initial conditions are hydrostatic in the CMG-GEM model (no fluid movement) and steady state in the MODFLOW model. Recharge takes place as well as ET and stream recharge. An accurate mass balance accounting for deep recharge is provided by the slow upwards movement of the water through the sediment pile and the top marine shale. It follows that only 4 of the 6 boundary conditions are identical in both models: no flow for the bottom, two side, and down-dip boundaries. The top boundary is handled by a “general head boundary” in the MODFLOW model whereas it becomes no-flow in the CMG-GEM model. The up-dip boundary is handled differently in the codes: through a complex interplay of shallow subsurface processes in MODFLOW and through a constant head condition in CMG-GEM. About 60 imaginary wells in both the Simsboro and Carrizo aquifers provide a means to numerically capture and measure the flux out of the system. Values for the constant head in the CMG-GEM model are either hydrostatic or provided by MODFLOW runs.

In order to somehow approximate changes brought by multiphase-flow processes to the MODFLOW model, we used modified permeability and porosity fields in the down-dip areas CO₂ is expected to sweep. Several analytical solutions provide an estimate of this extent (for example, Nordbotten et al. [4] and Hesse et al. [5]). The modified permeability field accounts for the change in conductivity following the change in viscosity and density of CO₂ relative to water (Table 1). Similarly, the modified porosity in the MODFLOW model input file accounts for the water residual saturation representing the pore space not available to CO₂. In addition, in CMG-GEM, we used a modified porosity on a cell by cell basis defined as the average sand porosity times the sand fraction to counter the coarseness of the grid and obtain a more realistic plume extent. The aquifer where CO₂ is injected is hundred to thousand feet thick and is represented by a single cell thickness in the MODFLOW model (refined into 4 sublayers in the CMG-GEM model). Inescapably such a large thickness of sediments will contain clay stringers and other flow barriers limiting the porosity volume contacted by the CO₂. The main result of the modified porosity is to obtain a more realistic CO₂ plume extent.

The relative permeability set used is semi-generic and has been used in other Gulf Coast settings. CMG-GEM models capillary hysteresis, important to model residual saturation trapping, and a value of 27.6% has been retained as maximum non wetting phase residual saturation. Water residual saturation was set at 13.7%. Capillary entry pressure is set high in the semi-confining layers to keep CO₂ within the injection formation and mimic a capillary seal. It follows that water is still able to flow through the seal and help in the attenuation of the pressure pulse impact to the fresh-water zone. MODFLOW does not handle

temperature variations directly and no assumption needs to be made relative to temperature. The temperature gradient option is used in the CMG-GEM model (a typical geothermal gradient of 30°C/km is used) but temperature values stay constant during a run. Neither code handles well water salinity changes and this lack of functionality is a limitation of both codes. In addition, we did not allow for dissolution of CO₂ into the aqueous phase. Other work suggests that a quarter to a third of the CO₂ can dissolve from the gas phase into the aqueous phase. Neglecting dissolution is more conservative relative to the pressure effects and also makes the comparison of the CMG-GEM model results with those of the MODFLOW model more consistent.

We also investigated the impact of the rock matrix compressibility on the modeling results. MODFLOW bundles water compressibility and matrix compressibility together into a parameter called storativity or, its intrinsic equivalent, storage coefficient. Storativity is accessible to field measurements through pump tests. CMG-GEM handles compressibility in a different manner and does not combine both media: compressibility values for gas and water are computed through the gas and water equation of state. Compressibility of the matrix is explicitly given either as a constant value across the field or possibly varying across cells but fixed for the duration of a run. For the purpose of this work, we extracted the base case matrix compressibility for input into the CMG-GEM model from the calibrated storativity field by subtracting the water compressibility at that depth.

Table 1. Changes relative to the original model (Dutton et al. [2])

Parameter -	MODFLOW	CMG-GEM
Porosity	Original porosity but modified locally to take impact of residual water saturation into account	Modified in each cell to account for shale stringers
Permeability	Original conductivity but modified locally to take density and viscosity of CO ₂ into account	Permeability computed from original conductivity assuming water at standard conditions
Relative permeability	N/A	Generic
Compressibility / Storativity	Original storativity	Matrix compressibility backcalculated from water compressibility and cell storativity
Temperature	N/A	Geothermal gradient
Initial conditions	Calibrated to pre-development conditions, including recharge and ET.	Hydrostatic (vertical equilibrium)
Injection	Fully penetrating	Only bottom 25% of injection formation thickness

3. Results and Conclusions

Nicot [1] concluded that large-scale CO₂ injection, at least in the Gulf Coast aquifers with a long run-up to the outcrop, will have, on average, minimal impacts on the fresh water section of those same aquifers. However, it is possible and was numerically observed, that flow barriers could locally focus displaced water and provoke undesirable effects. This conclusion is obviously a strong function of the size and geometry of the basin (Fig. 1b). Fig. 3a (from Nicot [1]) displays median, 90th percentile, and maximum water rise for the original, calibrated storativity of the MODFLOW model whereas Fig. 3b depicts values obtained with a storativity 10 times higher (in all formations). The maximum water rise shows more sensitivity to storativity (~5 and ~3.5 m for original and ×10 storativity, respectively) than the average water rise (between 0.5 and 1 m in both cases). The rising limb and decrease from the peak values are also more subdued through time when the system storativity is higher. The same observation can be made for evapotranspiration and, to a lesser extent, stream base flow (Fig. 4). These observations underline the importance of mudstones in attenuating the impact of the pressure pulse and of the existence of a mudstone/sandstone fraction trade-off. Abundant thick clean sandstones are a boon for injectivity but they would generate a possibly damaging pressure spike in the shallow subsurface whereas a significant amount of mudstones may decrease the theoretical capacity in some sense but allows for a decreased risk to the shallow subsurface; and this even if the tail end of the pressure pulse lasts longer because of the much attenuated peak. It follows that assessment of the compressibility of mudrocks in a basin could help significantly in gauging far-field risks. Comparison of Fig. 5 and 6 suggests that the operational volume initially targeted for modified porosity and permeability fields in the MODFLOW model was reasonably well-defined by the analytical solutions as supported by the CMG-GEM results.

The second objective of this paper was to determine the feasibility of using a simple single-phase flow code instead of a more complex multiphase flow code when modeling water displacement in the far-field. It appears that the assumption that local multiphase flow effects are negligible on the far-field is valid. We used the flux at the confined / unconfined transition zone as a metric to compare results from both models (Fig. 7) Results are in good agreement and fluxes are very similar, especially at larger storativity/matrix compressibility values. A likely explanation for the small deviation between the two models at lower storativity / matrix compressibility values is the ability of a larger storativity / compressibility to attenuate a pressure pulse sooner (Zhou et al. [6]; Oruganti and Bryant [7]), thus containing the CO₂ plume down-dip, where its density is high, for a longer time.

For lower matrix compressibility, CO₂ can migrate up-dip faster and becomes less dense in the process, thus displacing more water than anticipated by the constant value (700kg/m³) assumed in the MODFLOW model. Fig. 6b illustrates that CO₂ can migrate close to the up-dip boundary about 100 years after start of injection for the southwestern group of wells. It follows that single-phase flow models, with which most U.S. regulators are more comfortable, can be very useful in assessing far-field impacts.

Acknowledgments

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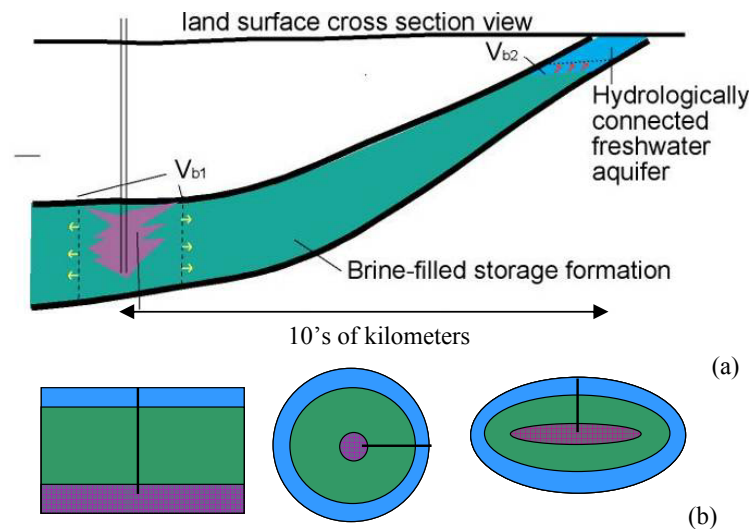


Figure 1. Conceptual model of water displacement at the basin scale: (a) cross sectional view of a single formation hydraulically connected from the deep subsurface to the outcrop (open system); water volume V_{b1} displaced while injecting CO₂ during time interval Δt pushes volume V_{b2} further up-dip (in general $V_{b1} \neq V_{b2}$). (b) map view of generalized basin outlines: Gulf Coast Basin, Illinois or Paris Basin, and Central Valley, CA Basin, respectively.

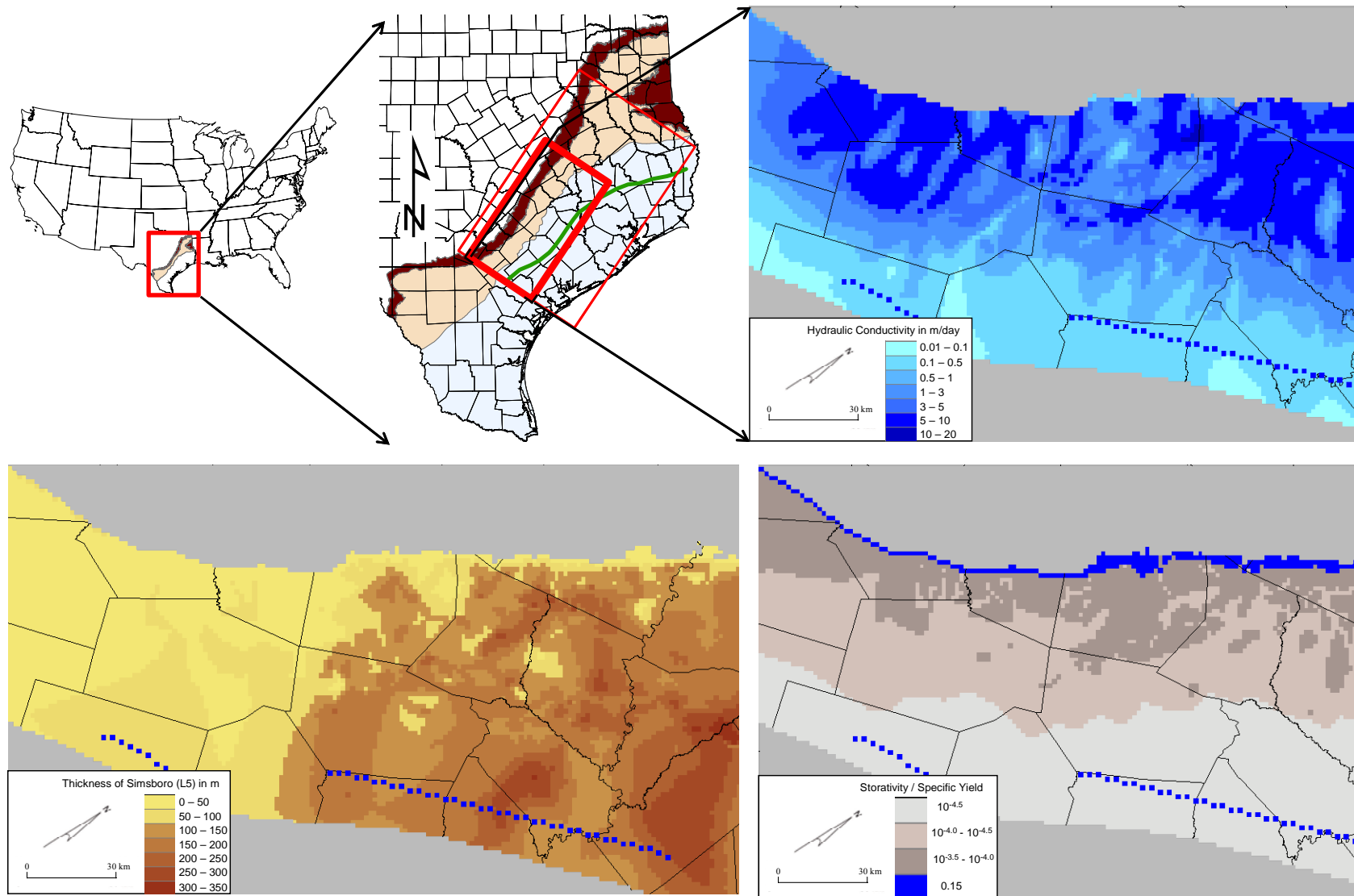


Figure 2. Location of the Carrizo-Wilcox aquifer system in Texas and map views of distribution of hydraulic conductivity, thickness, and storativity of the Simsboro aquifer.

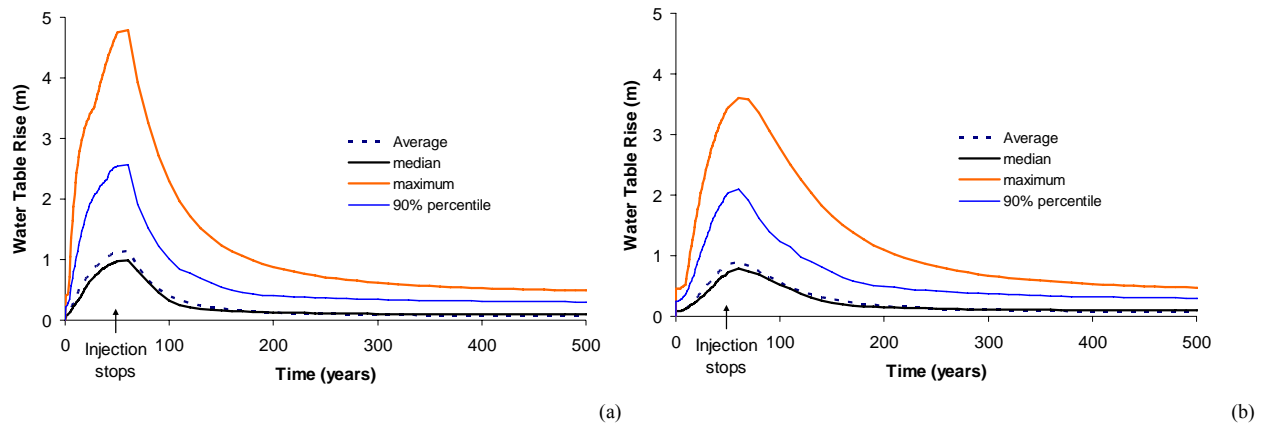


Figure 3. Impact of storativity on water level rise on outcrop: (a) original storativity; (b) increase by a factor of 10.

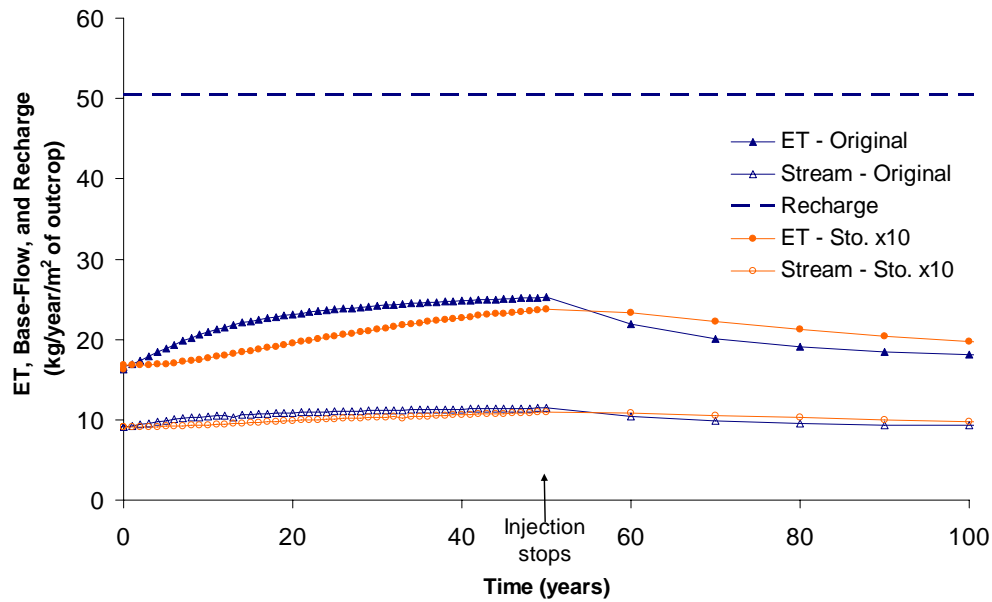


Figure 4. Comparison of ET and stream leakage MODFLOW outputs for 2 storativity values (original and increased by a factor 10)

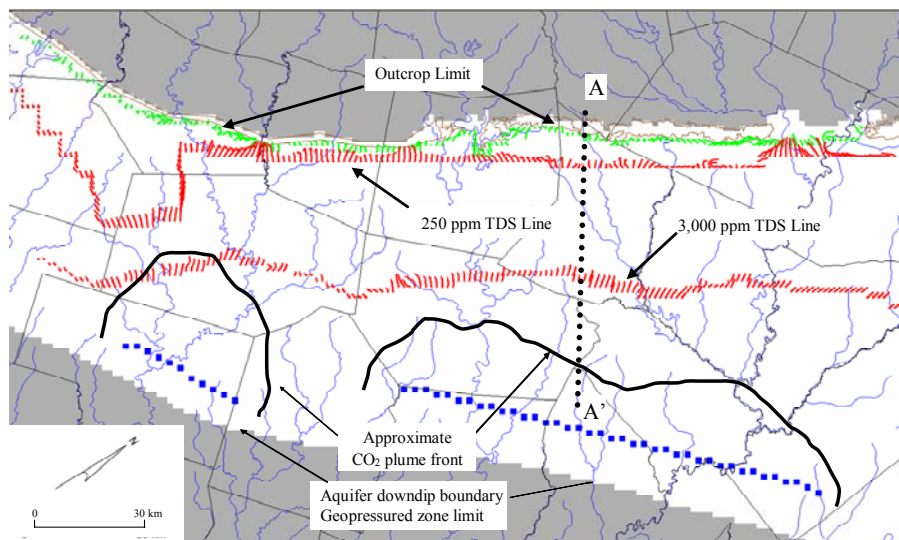


Figure 5. Approximate location of CO₂ plume as given by analytical solutions at the end of injection (thick black line) and vectors depicting translation of targeted salinity contour lines (3,000 and 250 mg/L Total Dissolved Solids) as given in the MODFLOW model. More explanations given in Nicot [1].

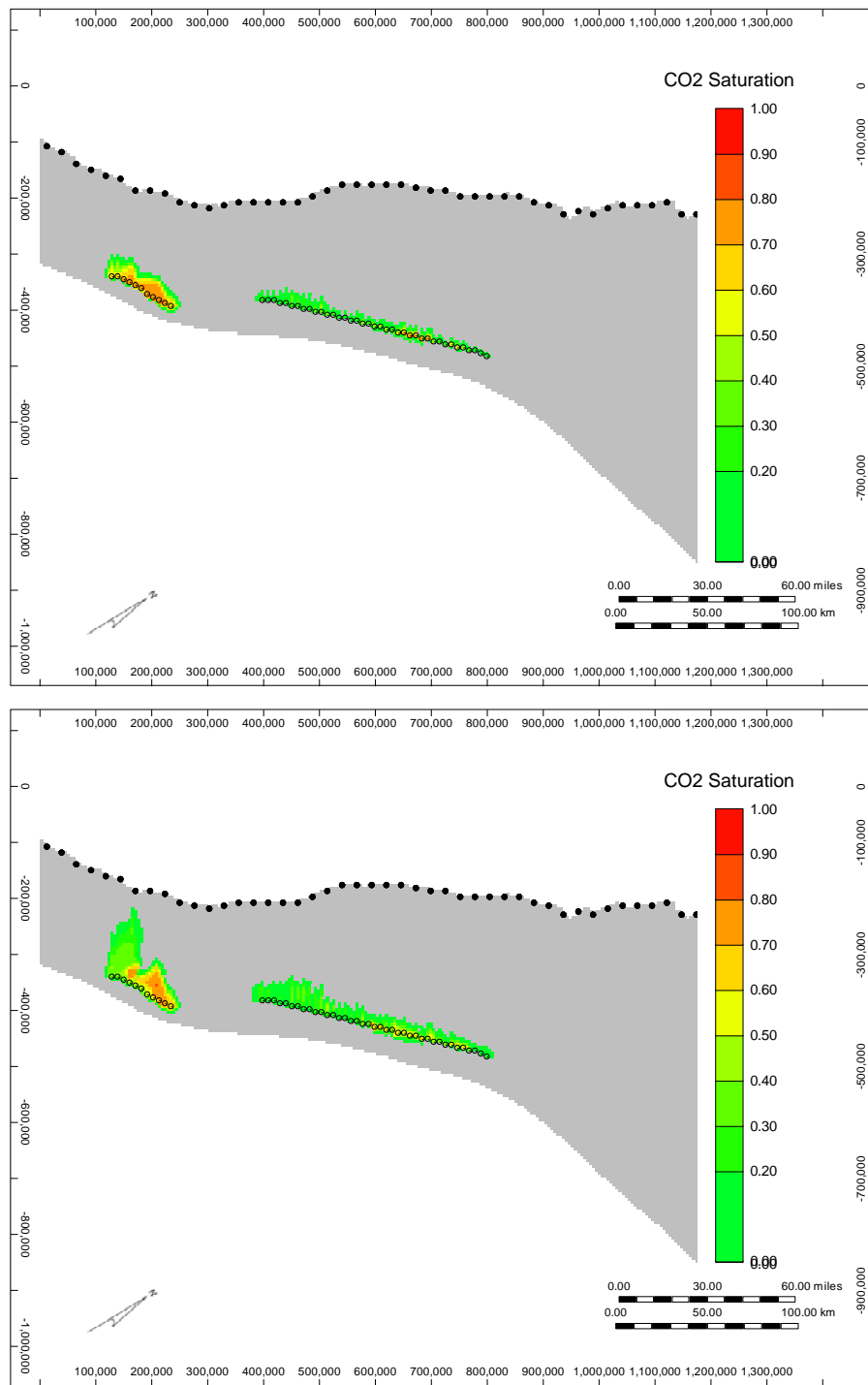


Figure 6. CO₂ plume at 50 (top) and ~100 (bottom) years after start of injection as given by CMG-GEM, to be compared to approximate edge of CO₂ plume as given by MODFLOW (Fig. 5).

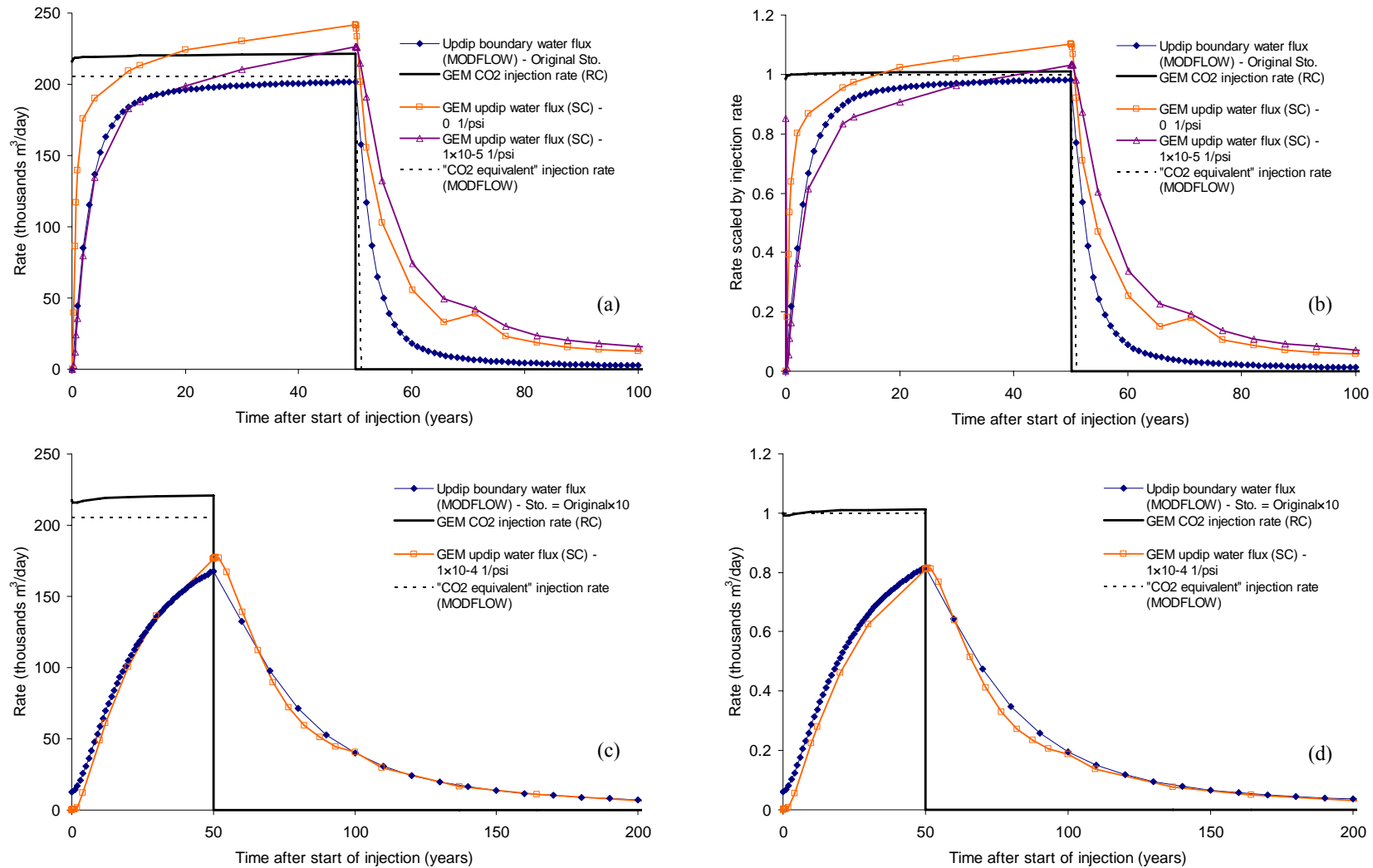


Figure 7. Comparison of MODFLOW and CMG-GEM fluxes at the updip boundary of the model for different storativity/compressibility values. Left column represents model outputs whereas right column represents model outputs scaled by the average injection rate. Top row displays comparison of MODFLOW total flux for the original storativity with 2 CMG-GEM total flux curves for 2 different matrix compressibility values whereas bottom row displays same comparison but for storativity and matrix compressibility increased by a factor $\times 10$.